

Manipulating unpaired Majorana fermions in a quantum spin chain

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We analyse an exactly solvable spin-1/2 chain which is a generalised version of Kitaev's honeycomb model. We show that every state of the system has a $2^{N/4}$ fold degeneracy, where N is the number of sites. We present analytic solutions for the zero energy modes of the Majorana fermions. Localised, unpaired Majorana modes occur even in the bulk of the chain and they are bound to kink (anti-kink) Z_2 flux configurations. The unpaired Majorana modes can therefore be created and manipulated if the Z_2 flux configurations can be controlled. We delineate the regions in parameter space for homogenous chains where the zero modes occur. We further show that there is a large parameter space for inhomogenous chains where the unpaired modes occur and that their wavefunctions can be tuned if the couplings of the model can be tuned.

I. INTRODUCTION

The idea of topological quantum computation as a way to incorporate fault tolerance at the hardware level has been getting a lot of attention recently¹. In this scheme, qubits are non-abelian anyons and the braiding operations on them implement quantum gates. One of the simplest class of non-abelian anyons are realised in systems with unpaired Majorana fermions (UMF)². In a fermionic system with N zero energy modes, there are 2^N Majorana modes. If these $2N$ modes can be independently moved around each other, then the geometric phases picked up correspond to a non-abelian representation of the braid group. Thus it is of interest to study physically realisable systems where UMF exist and can be manipulated.

Non-abelian anyons are theoretically predicted to occur in certain fractional quantum Hall states like $\nu = 5/2$ ³. There is also theoretical work showing how they could be realised in quantum circuits⁴. In this context, Kitaev presented a remarkable solvable spin-1/2 model on a honeycomb lattice⁵ which realises non-abelian anyons made up of UMF. The model can be written in terms of Majorana fermions in the background of Z_2 gauge fields. This fermionisation procedure is very similar to that proposed in the context of the resonating valence bond (RVB) theory⁶. The crucial difference is that in Kitaev's honeycomb model, the gauge fields are constants of motion, hence the RVB type mean field theory is exact and the problem reduces to solving a theory of non-interacting Majorana fermions in the background of static Z_2 gauge field configurations. Kitaev showed that the ground state is the flux free configuration. The model has a phase which is characterised by a topological invariant, the Chern number, being equal to ± 1 . In this phase there are UMF trapped to each vortex (a Z_2 flux). Thus if vortices can be created and manipulated, it is possible to braid the UMF. However, the Z_2 flux operator is a 6-spin operator and thus may not be easy to realise in practice.

Kitaev's honeycomb model can be generalised to a variety of other lattices. It can be constructed on any lattice

with coordination number three, if all the bonds can be coloured using three colours. It has been shown that all such models can be realised in cold atom systems⁷ and using quantum circuits⁸.

In paper we present a one dimensional generalisation of Kitaev's honeycomb model which we call the tetrahedral chain (TC) and analyse its zero energy modes in detail. One dimensional models with UMF at the edges have been studied earlier^{9,10}. The new feature of the TC is that the wavefunctions of the UMF not necessarily peaked at the edges of the chain but can be peaked anywhere in the bulk. As we will show, they are trapped to kink and anti-kink flux configurations and can be moved by tuning the flux configuration. Further, by tuning the coupling constants, their wavefunctions, which we obtain analytically, can also be tuned.

The rest of this paper is organised as follows. In section II we present the model and its conserved quantities. Section III describes the Jordan-Wigner transformation which enables us to rewrite the theory in terms of Majorana fermions hopping in the background of static Z_2 gauge field configurations. The diagonalisation of the Majorana fermion problem is described in section IV and the numerical calculations to determine the ground state flux configurations are presented in section V. Section VI gives an analytic proof of the degeneracy of the eigenstates that we find numerically. The dependence of the gap as a function of the couplings is computed in section VII and a gapless line in the parameter space is identified. Section VIII contains a detailed analysis of the zero-modes of the Majorana fermions. We summarise our results and discuss them in the concluding section IX.

II. THE TETRAHEDRAL MODEL

The chain we define our model on is shown in Fig. 1. There are four sites per unit cell which are labelled as

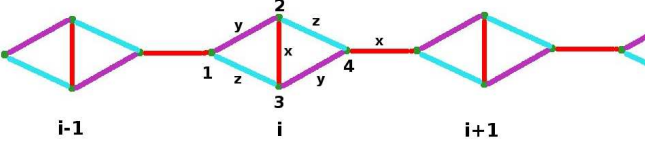


FIG. 1: The tetrahedral Kitaev chain. There are four sites per unit cell. The x, y and z bonds are as indicated.

shown in the figure. The hamiltonian is,

$$H = \sum_i (J_x (\sigma_{i-1,4}^x \sigma_{i,1}^x + \sigma_{i,2}^x \sigma_{i,3}^x) + J_y (\sigma_{i,1}^y \sigma_{i,2}^y + \sigma_{i,3}^y \sigma_{i,4}^y) + J_z (\sigma_{i,1}^z \sigma_{i,3}^z + \sigma_{i,2}^z \sigma_{i,4}^z)) \quad (1)$$

There are two triangular plaquettes in each unit cell and a conserved Z_2 flux associated with each of them. The flux operators are,

$$W_i^L = \sigma_{i,1}^x \sigma_{i,2}^z \sigma_{i,3}^y \quad W_i^R = \sigma_{i,4}^x \sigma_{i,3}^z \sigma_{i,2}^y \quad (2)$$

As in Kitaev's honeycomb model, these quantities are conserved as a consequence of a local spin rotation symmetry of the model. Namely, a π rotation on each site of a plaquette about the direction of the outgoing bond.

Apart from these local conserved quantities there are also three global quantities which are conserved as a consequence the fact that a global π rotation about each of the three axes is a symmetry of the model. We denote these by,

$$\Sigma^a \equiv e^{i\frac{\pi}{2} \sum_{i,a} \sigma_{i,a}^a} \quad (3)$$

It can be verified that Σ^x is the product of the fluxes of all the plaquettes,

$$\Sigma^x = \prod_i (W_i^L W_i^R) \quad (4)$$

III. FERMIONISATION

We express the hamiltonian in terms of Majorana fermions using the Jordan-Wigner transformation. We choose the Jordan-Wigner path to go along the x and the y bonds from left to right. At every site we have two bonds that are tangential to the path. We denote the incoming bond by t_1 . This is the x -bond on the sublattices 1, 3 and y -bond on sublattices 2,4. The outgoing bond, corresponding to y on sublattices 1,3 and x on sublattices 2,4, is denoted by t_2 . The third bond on each site which is normal to the path is denoted by n with the sign defined by $\hat{n} = \hat{t}_1 \times \hat{t}_2$. With our choice of path, the normal bond is z for sublattices 1,3 and $-z$ for sublattices 2,4.

With these definitions the two Majorana fermions at each site are defined as,

$$\xi_{i,\alpha} = \sigma_{i,\alpha}^{t_1} \prod_{j<i} \left(\prod_{\beta<\alpha} \sigma_{j,\beta}^n \right) \quad (5)$$

$$\eta_{i,\alpha} = \sigma_{i,\alpha}^{t_2} \prod_{j<i} \left(\prod_{\beta<\alpha} \sigma_{j,\beta}^n \right) \quad (6)$$

The hamiltonian can be expressed in terms of the Majorana fermions defined above,

$$H = \sum_i (J_x (i\xi_{i-1,4}\xi_{i,1} + i\xi_{i,2}\xi_{i,3}) + J_y (i\xi_{i,1}\xi_{i,2} + i\xi_{i,3}\xi_{i,4}) + J_z (-iu_i^L \xi_{i,1}\xi_{i,3} + iu_i^R \xi_{i,2}\xi_{i,4})) \quad (7)$$

$$(8)$$

where the link fields, $u_i^{L(R)}$ are defined as,

$$u_i^L \equiv i\eta_{i,3}\eta_{i,1} \quad u_i^R \equiv i\eta_{i,2}\eta_{i,4} \quad (9)$$

It is easy to see that the link fields are conserved quantities. Thus, as expected for a generalised Kitaev model, the theory gets written in terms of Majorana fermions with nearest neighbour hopping in the background of conserved Z_2 gauge fields with the gauge fixing condition that the gauge fields on the x and y bonds are equal to +1. It is easy to check that in this gauge the two flux operators are proportional to the link fields,

$$u_i^L \equiv i\eta_{i,3}\eta_{i,1} = W_i^L \quad u_i^R \equiv i\eta_{i,2}\eta_{i,4} = W_i^R \quad (10)$$

It is instructive to express the three global conserved quantities, Σ^a in terms of the fermionic variables. We have,

$$\Sigma^x = \prod_i (\eta_{i,1}\eta_{i,2}\eta_{i,3}\eta_{i,4}) \quad (11)$$

$$\Sigma^y = \prod_i (\xi_{i,1}\xi_{i,2}\xi_{i,3}\xi_{i,4}) \quad (12)$$

$$\Sigma^z = \Sigma^x \Sigma^y \quad (13)$$

We will refer to Σ^x as the flux number and Σ^y as the Majorana number.

IV. DIAGONALISATION

The hamiltonian can be diagonalised in the standard way. We write the eigenstates as direct products of states in the η fermion sector, $|\mathcal{G}\rangle$, which we will refer to as the gauge sector and states in the ξ fermion sector, $|\mathcal{M}\rangle$, which we call the matter sector. We choose the states in the gauge sector to be the simultaneous eigenstates of the Z_2 flux operators, i.e $|\mathcal{G}\rangle = |\{w_i^L, w_i^R\}\rangle$, where

$$u_i^{L(R)} |\{w_i^L, w_i^R\}\rangle = w_i^{L(R)} |\{w_i^L, w_i^R\}\rangle \quad (14)$$

We then have

$$H [u_i^L, u_i^R] |\mathcal{M}\rangle |\{w_i^L, w_i^R\}\rangle = H [w_i^L, w_i^R] |\mathcal{M}\rangle |\{w_i^L, w_i^R\}\rangle \quad (15)$$

The problem reduces to finding the eigenstates of the quadratic hamiltonian of the ξ fermions in the background of the gauge field configuration $\{w_i^L, w_i^R\}$. The normal modes are given by the solution of the eigenvalue equation,

$$\sum_{j\beta} A_{i\alpha,j\beta} \phi_{j\beta}^n = \epsilon_n \phi_{i\alpha}^n \quad (16)$$

where $A = T + V$ is a purely imaginary anti-symmetric matrix,

$$T_{i,j} = iJ_x \begin{pmatrix} 0 & 0 & 0 & -\delta_{i-1,j} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \delta_{i+1,j} & 0 & 0 & 0 \end{pmatrix} \quad (17)$$

$$V_{i,j} = i\delta_{i,j} \begin{pmatrix} 0 & J_y & -J_z w_i^L & 0 \\ -J_y & 0 & J_x & J_z w_i^R \\ J_z w_i^L & -J_x & 0 & J_y \\ 0 & -J_z w_i^R & -J_y & 0 \end{pmatrix} \quad (18)$$

The eigenvalues come in pairs, $\pm\epsilon_n$. So we can always choose ϵ_n to be positive. The eigenvectors corresponding to the positive and negative eigenvalues are complex conjugates. Denoting the real and imaginary parts of the eigenvectors as $\phi^{nR(I)}$, we expand the ξ fermions as,

$$\xi_{i,\alpha} = \sum_n a_n \phi_{i,\alpha}^{nR} + b_n \phi_{i,\alpha}^{nI} \quad (19)$$

a_n and b_n are also Majorana fermions. The diagonal form of the hamiltonian is then,

$$H = \sum_n \epsilon_n i b_n a_n \quad (20)$$

The ground state energy is the one where all the operators $i b_n a_n$ are diagonal and equal to -1. The ground state energy is,

$$E_0 = - \sum_n \epsilon_n \quad (21)$$

A. Boundary Conditions

We will be analysing the system with periodic (PBC) and open boundary conditions (OBC). The latter case is straightforward. The fermionic hamiltonian is exactly of the form given in equation (7) with $i = 1, \dots, N$, where N is the number of unit cells. The fermionic modes have to be solved with the boundary conditions

$$\phi_{0,a} = \phi_{N+1,a} = 0 \quad (22)$$

PBC is a little more subtle. As is standard in Jordan-Wigner transformations, the term in the hamiltonian for the link $i = N$ to $i = 1$ is,

$$H_{N,0} = J_x \Sigma^z i \xi_{1,1} \xi_{N,4} \quad (23)$$

Σ^z is a conserved quantity and can hence be chosen to be diagonal. The fermionic modes have to be solved with periodic boundary conditions for states with $\Sigma^z = +1$ and with anti-periodic boundary conditions for states with $\Sigma^z = -1$. Namely,

$$\phi_{N+1,\alpha} = p \phi_{1,\alpha} \quad (24)$$

where $p = \pm 1$ is the eigenvalue of Σ^z .

V. THE NUMERICAL SOLUTION

We have solved eigenvalue problem numerically for a chain with N unit cells and open boundary conditions for $N \leq 5$. Each unit cell has 4 possible flux configurations making a total of 4^N . We computed the single particle spectrum for each flux configuration and calculated the lowest total energy state for the range of values $J_x = 1.0$, $J_y = 0.1 - 10$, $J_z = 0.1 - 10$ (in the steps of 0.2).

We find that the ground state is 2^N fold degenerate for all values of the parameters. This degeneracy comes from the fact that the single particle spectrum depends only on the values of the product, $w_i \equiv w_i^L w_i^R$, and not on their individual values. i.e the spectrum only sees the total flux passing through each unit cell which is the product of the values of the fluxes passing through the two triangular plaquettes that make up the unit cell.

The ground states correspond to the translationally invariant, $w_i = 1$, flux configurations.

VI. THE DEGENERACY OF THE STATES

As mentioned above, we find that the spectrum in each sector is 2^N fold degenerate. This degeneracy is due to the fact that the energy eigenvalues depend only on the total flux in the unit cell, namely $w_i \equiv w_i^L w_i^R$ and not on the individual fluxes, w_i^L and w_i^R . In the remaining part of this section, we will give an analytic proof of this 2^N fold degeneracy of all the states.

This degeneracy is related to but not the same as the 4^N degeneracy that occurs in the simple Kitaev chain, the $J_z = 0$ limit of our model. In this case the degeneracy is easy to understand. The gauge fields do not occur at all in the hamiltonian. Thus each state is 4^N degenerate corresponding to all the states in the gauge sector. The extra z -bond terms in our model lift this degeneracy only partially.

At $J_y = J_z$, the degeneracy can be understood in terms of a local symmetry. It consists of interchanging the spins at sublattice 2 and 3 in any unit cell and then performing a $\pi/2$ rotation about the x -axis on all the spins in that

unit cell. The operator that implements this transformation is,

$$P_i \equiv \left(\frac{\vec{\sigma}_{i2} \cdot \vec{\sigma}_{i3} + 1}{2} \right) e^{i\frac{\pi}{4} \sum_{\alpha=1}^4 \sigma_{i\alpha}^x} \quad (25)$$

It is easy to verify that the P_i 's commute with the hamiltonian, However P_i flips the sign of the two flux operators in the unit cell,

$$P_i W_i^{L(R)} P_i = -W_i^{L(R)}, \quad P_i^2 = W_i^L W_i^R \quad (26)$$

Thus it changes the flux configuration while conserving the total flux through the unit cell. Since it also does not change the energy eigenvalue, it follows that every eigenstate of the hamiltonian is 2^N fold degenerate.

However, we numerically observe that the degeneracy persists even when $J_y \neq J_z$. We will now give a proof for the degeneracy which is valid at all couplings. We note that in equation (16), $\phi_{i,2}$ and $\phi_{i,3}$ couple only to sites within the unit cell. We express them in terms of $\phi_{i,1}$ and $\phi_{i,4}$ and obtain an eigenvalue equation for these quantities. We are then able to show that the eigenvalues depend only on w_i .

We define the two component column vectors,

$$\chi_i \equiv \begin{pmatrix} \phi_{i,1} \\ \phi_{i,4} \end{pmatrix} \quad \psi_i \equiv \begin{pmatrix} \phi_{i,2} \\ \phi_{i,3} \end{pmatrix} \quad (27)$$

and the matrices,

$$T_{ij} = i\delta_{i-1,j} \begin{pmatrix} 0 & -J_x \\ 0 & 0 \end{pmatrix} + i\delta_{i+1,j} \begin{pmatrix} 0 & 0 \\ J_x & 0 \end{pmatrix} \quad (28)$$

$$U_{ij} = i\delta_{i,j} \begin{pmatrix} J_y & J_z w_i^L \\ J_z w_i^R & -J_y \end{pmatrix} \quad (29)$$

The eigenvalue equations (16) can be written as,

$$\begin{pmatrix} T & U \\ U^\dagger & J_x \tau^2 \end{pmatrix} \begin{pmatrix} \chi \\ \psi \end{pmatrix} = \epsilon \begin{pmatrix} \chi \\ \psi \end{pmatrix} \quad (30)$$

where τ^a , $a = 1, 2, 3$ are the Pauli matrices. ψ can be eliminated from the equations to get,

$$\left(T + U \frac{1}{\epsilon - J_x \tau^2} U^\dagger \right) \chi = \epsilon \chi \quad (31)$$

The equations can be explicitly written as,

$$-iJ_x \phi_{i-1,4} + c_i e^{i\alpha_i} \phi_{i,4} = \lambda \phi_{i,1} \quad (32)$$

$$iJ_x \phi_{i+1,1} + c_i e^{-i\alpha_i} \phi_{i,1} = \lambda \phi_{i,4} \quad (33)$$

where,

$$c_i = \sqrt{\frac{J_x^2(J_y^2 + J_z^2)^2 + 2J_z^2 J_y^2(\epsilon^2 - J_x^2)(1 - w_i)}{(\epsilon^2 - J_x^2)^2}} \quad (34)$$

$$\alpha_i = \tan^{-1} \left(\frac{\epsilon J_y J_z}{J_x(J_y^2 + J_z^2 w_i)} (w_i^R - w_i^L) \right) \quad (35)$$

$$\lambda = \epsilon \left(1 - \frac{J_y^2 + J_z^2}{\epsilon^2 - J_x^2} \right) \quad (36)$$

When these equations are solved for λ , they will yield an equation for ϵ . We now make a transformation,

$$\phi_{i,1} \rightarrow e^{i\theta_i} \phi_{i,1} \quad (37)$$

$$\phi_{i,4} \rightarrow e^{i\theta_{i+1}} \phi_{i,4} \quad (38)$$

$$\theta_i = -\sum_{j<i} \left(\alpha_j + \frac{\pi}{2} \right) \quad (39)$$

This gets rid of the phases in equations (32) and (33) which become,

$$-iJ_x \phi_{i-1,4} - ic_i \phi_{i,4} = \lambda \phi_{i,1} \quad (40)$$

$$iJ_x \phi_{i+1,1} + ic_i \phi_{i,1} = \lambda \phi_{i,4} \quad (41)$$

Since c_i depends only on w_i and not on w_i^L and w_i^R individually, λ and hence ϵ depends only on the w_i . Thus the energy eigenvalues depend only on the total flux passing through the unit cell.

This result is true for all values of J_x, J_y and J_z . Note that when $J_z = 0$, equation (34) implies that c_i is independent of w_i also. Thus the 4^N fold degeneracy of the simple Kitaev chain is recovered in this limit.

VII. THE GROUND STATES AND GAPS

As we have mentioned earlier our numerical results show that the translationally invariant fluxes through the unit cells, namely $w_i = 1$ is one of the ground states of the model. The fermionic problem is easy to solve analytically for these flux configurations and therefore the energy of the $w = 1$ configuration can be compared to that of the $w = -1$ configuration in the thermodynamic limit.

If $w_i = w$, then c_i in equations (40, 41) are independent of i , $c_i = c$. The equations can be solved by Fourier transforms,

$$\phi_{i,a} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{iki} \phi_a(k) \quad (42)$$

$$\phi_a(k) = \sum_i e^{-iki} \phi_{i,a} \quad (43)$$

λ is then given by the eigenvalues of the following matrix,

$$\begin{pmatrix} 0 & -i(c + J_x e^{-ik}) \\ i(c + J_x e^{-ik}) & 0 \end{pmatrix} \quad (44)$$

namely,

$$\lambda = \pm \sqrt{c^2 + J_x^2 + 2cJ_x \cos k} \quad (45)$$

Along with equation (36) this yields an equation for the four energy bands. We have solved for this energy bands and have computed the gap for $0 < J_y, J_z < 10$ and $J_x = 1$.

The calculations confirm that the $w_i = +1$ sector has a lower ground state energy than the $w_i = -1$ sector. The

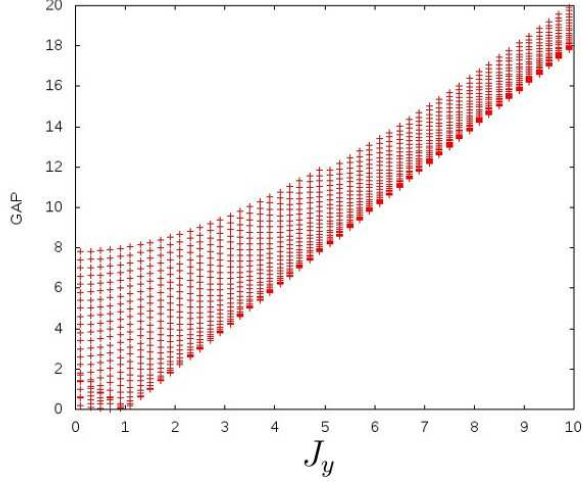


FIG. 2: The gap plotted against J_y for $J_x = 1$ and values of J_z varying in the range $0 < J_z < 10$. It can be seen that the $J_y < 1$ region is gapless for some value of J_z .

fermionic gap is twice the value of the lowest single particle energy eigenvalue. This is shown in Figure 2 where the gap is plotted against J_y for different values of J_z . The $J_y < 1$ region is clearly gapless. It is interesting that when we plot the gap as a function of $J \equiv \sqrt{J_y^2 + J_z^2}$, all the points fall on the straight line as shown in Fig. 3. This can be shown analytically since the expression in equation (34) simplifies considerably at $w_i = 1$. It is then easy to show that the energy eigenvalues are given by,

$$\epsilon^2 = J^2 + 1 \pm 2J \cos\left(\frac{k}{2}\right) \quad (46)$$

The gap is thus given by,

$$\Delta = 2J_x |J - 1| \quad (47)$$

The circle in the parameter space, $J_x^2 = J_y^2 + J_z^2$ is therefore gapless.

VIII. ZERO MODES AND KINKS

We will now analyse the zero energy modes of the Majorana fermions. When $\epsilon = 0$, we have $\lambda = 0$ and hence the equations (40) and (41) decouple and become very simple,

$$J_x \phi_{i+1,1} + \frac{J_y^2 + w_i J_z^2}{J_x} \phi_{i,1} = 0 \quad (48)$$

$$J_x \phi_{i-1,4} + \frac{J_y^2 + w_i J_z^2}{J_x} \phi_{i,4} = 0 \quad (49)$$

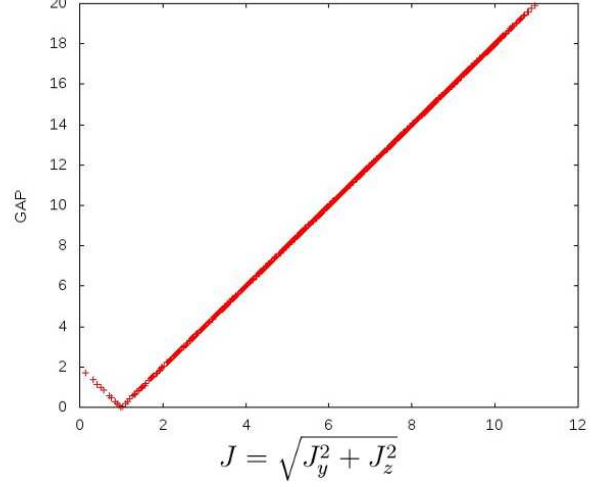


FIG. 3: The gap plotted against $J \equiv \sqrt{J_y^2 + J_z^2}$. The points fall on straight lines with slopes ± 2

These recursion relations can be formally solved,

$$\phi_{i,1} = \prod_{j<i} \left(\frac{J_y^2 + w_j J_z^2}{J_x^2} \right) \phi_1 \quad (50)$$

$$\phi_{i,4} = \prod_{j>i} \left(\frac{J_y^2 + w_j J_z^2}{J_x^2} \right) \phi_4 \quad (51)$$

Where $\phi_{1(4)}$ are arbitrary constants. Thus, there are two formal solutions for every set of values of the parameters and every flux configuration. One with $\phi_{i,1} \neq 0$ and $\phi_{i,4} = 0$ which we denote by ϕ^+ and the other with $\phi_{i,1} = 0$ and $\phi_{i,4} \neq 0$ which we denote by ϕ^- .

However, the boundary conditions that the modes have to satisfy will pick out certain flux configurations for each point in the parameter space. We will analyse the situation for the cases of periodic boundary conditions (PBC) and open boundary conditions (OBC).

A. Periodic Boundary Conditions

We consider a chain with N unit cells. As discussed in equation (24), PBC will imply that,

$$\phi_{N+1,a} = p \phi_{1,a} \quad (52)$$

Equations (50), (51) and (52) imply

$$\prod_{i=1}^N \left(\frac{J_y^2 + w_i J_z^2}{J_x^2} \right) = p \quad (53)$$

Consider the general case where $M \leq N$ of the w_i 's are equal to -1 and $N - M$ of them are $+1$. We will refer to such configurations as M -defect configurations. Equation (53) gets written as,

$$\left(\frac{J_y^2 - J_z^2}{J_y^2 + J_z^2} \right)^M = p \left(\frac{J_x^2}{J_y^2 + J_z^2} \right)^N \quad (54)$$

When $M = 0$, we have only have solutions on the circle of radius J_x in the $J_y - J_z$ plane. Note that $M = 0$ is the translationally invariant ground state flux configuration. Thus this result implies that the model is gapless only on the circle, consistent with equation (47).

When $M > 0$, since the LHS of equation (54) is less than 1, no zero modes exist within the circle of radius J_x . Outside this circle, for every even M there are two directions where equation (54) is satisfied with $p = +1$. One direction where $J_y > J_z$ and the other where $J_z > J_y$. For odd M , the $J_y > J_z$ solution exists for $p = +1$ and the $J_y < J_z$ solution for $p = -1$.

Thus for every N there are a discrete set of points outside the circle which support zero energy modes. In the thermodynamic limit of $N \rightarrow \infty$, N/M can take all values from 1 to ∞ . In this limit, all the points outside the circle in the range, $J_x^2 \leq |J_y^2 - J_z^2| \leq 0$ support zero energy modes. This region is shown for $J_x = 1$ in Fig. 4

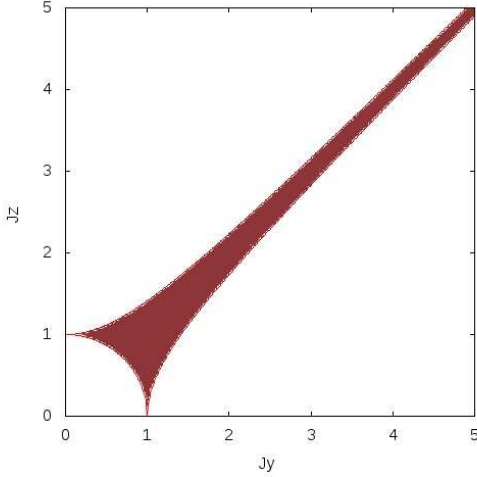


FIG. 4: The region in the $J_y - J_z$ plane at $J_x = 1$ that supports zero energy modes

Consider the cases when the M defects are in adjoining unit cells, say from $i = 1$ to $i = M$. We will call this a kink-antikink configuration. We define polar coordinates in the $J_y - J_z$ plane,

$$J \equiv \sqrt{J_y^2 + J_z^2}, \quad \gamma = \tan^{-1} \left(\frac{J_z}{J_y} \right) \quad (55)$$

The unnormalised wave functions of the two zero modes are,

$$\phi_{i,1}^+ = J^{2(i-1)} \quad i \leq M+1 \quad (56)$$

$$= J 2^{(i-1)} (\cos 2\gamma)^{i+1-M} \quad i > M+1 \quad (57)$$

$$\phi_{i,4}^+ = 0 \quad (58)$$

$$\phi_{i,4}^- = J^{-2(i-1)} \quad i \leq M+1 \quad (59)$$

$$= J^{-2(i-1)} (\cos 2\gamma)^{-(i+1-M)} \quad i > M+1 \quad (60)$$

$$\phi_{i,1}^- = 0 \quad (61)$$

$\phi_{i,2}^\pm$ and $\phi_{i,3}^\pm$ are given in terms of $\phi_{i,1}^\pm$ and $\phi_{i,4}^\pm$,

$$\phi_{i,2}^\pm = \frac{1}{J_x} (J_y \phi_{i,1}^\pm - w_i^R J_z \phi_{i,4}^\pm) \quad (62)$$

$$\phi_{i,3}^\pm = \frac{1}{J_x} (w_i^L J_z \phi_{i,1}^\pm + J_y \phi_{i,4}^\pm) \quad (63)$$

It can be seen that ϕ^+ is peaked at $i = M$ and is minimum at $i = 1$ whereas ϕ^- is peaked at $i = 1$ and has a minimum at $i = M$. Thus we have one Majorana mode localised at the location of the kink and another at the location of the antikink. When M is large these are well separated. Thus the situation is similar to Kitaev's honeycomb model with kinks and antikinks playing the role of the vortices. If the flux configuration can be manipulated, then so can the Majorana modes trapped to them.

B. Open Boundary Conditions

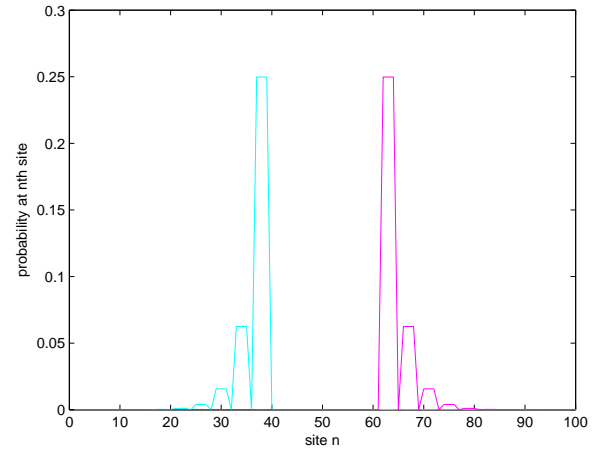


FIG. 5: The wavefunctions of the two Majorana zero modes for $N = 25$, $M = 7$ with open boundary conditions.

We now consider open chains with N unit cells. We then need to solve equations (48) and (49) with the boundary conditions in equation (22). From the solutions in equation (50) and (51), we see that the above boundary conditions have non trivial solutions if and only if at least one of the factors in the products on the RHS of the equations is zero. This is only possible when $|J_y| = |J_z|$. Thus zero modes exist in this case only at $\gamma = \pi/4$. At these points, the zero modes are similar the ones in the PBC case except that the wavefunctions strictly vanish in the region between the kink and the antikink. Namely, if we consider a flux configuration with $w_i = -1$, $i_i \leq i < i_i + M$, then the wavefunctions are

given by,

$$\phi_{i,1}^+ = J^{2(i-1)} \quad i \leq i_1 \quad (64)$$

$$= 0 \quad i > i_1 \quad (65)$$

$$\phi_{i,4}^+ = 0 \quad (66)$$

$$\phi_{i,4}^- = J^{-2(i-1)} \quad i > i_1 + M \quad (67)$$

$$= 0 \quad i > M + 1 \quad (68)$$

$$\phi_{i,1}^- = 0 \quad (69)$$

$\phi_{i,2}^\pm$ and $\phi_{i,3}^\pm$ are given in terms of $\phi_{i,1}^\pm$ and $\phi_{i,4}^\pm$ as before. These wavefunctions are shown in Fig. 5 for $N = 25$ and $M = 7$.

C. Inhomogenous chains

The solutions for the zero mode equations (48) and (49) hold even for the case of inhomogenous chains where the coupling constants J_y and J_z depend on i . The equations then read

$$J_x \phi_{i+1,1} + \frac{J_y^2 + w_i J_z^2}{J_x} \phi_{i,1} = 0 \quad (70)$$

$$J_x \phi_{i-1,4} + \frac{J_y^2 + w_i J_z^2}{J_x} \phi_{i,4} = 0 \quad (71)$$

These solution to these recursion relations is exactly the same as the case of the homogenous chain with i dependent $J_{y(z)}$.

$$\phi_{i,1} = \prod_{j < i} \left(\frac{J_{yj}^2 + w_j J_{zj}^2}{J_x^2} \right) \phi_1 \quad (72)$$

$$\phi_{i,4} = \prod_{j > i} \left(\frac{J_{yj}^2 + w_j J_{zj}^2}{J_x^2} \right) \phi_4 \quad (73)$$

It is clear that by tuning the values of the site dependent couplings, a large variety of zero mode wavefunctions can be engineered.

D. Tuning the flux configuration

We can add the following “chemical potential” term for the conserved flux operators,

$$H_\mu = \sum_i (\mu_i^L W_i^L + \mu_i^R W_i^R) \quad (74)$$

This term will not change the eigenstates but will alter the energy eigenvalues. If the $\mu_i^{L(R)}$ can be tuned,

then any particular flux configurations can be made the ground state.

However it is still not known how to engineer these 3-spin operators in the physical realisations of the model in cold atom systems or in quantum circuits.

IX. CONCLUSIONS

To summarize, we have analysed an exactly solvable spin-1/2 chain which we call a tetrahedral chain. This model is a generalization of Kitaev’s honeycomb lattice model. Like the honeycomb model, this model too has three coupling constants, J_x , J_y and J_z . One of them can be scaled away, so without loss of generality, we can set $J_x = 1$.

The model has conserved Z_2 fluxes on every triangular plaquette, namely two fluxes per unit cell. We denote the values of these fluxes by $w_i^{L(R)}$. The fermionic spectrum in the background of the flux configuration depends only on the total flux in the unit cell, $w_i \equiv w_i^L w_i^R$. Consequently, every eigenstate of the model is 2^N fold degenerate, where N is the number of unit cells.

The ground state flux configurations of the model are the ones with $w_i = 1$. The model is gapless on the unit circle in the $J_y - J_x$ plane and is gapped everywhere else.

We have found simple analytic solutions for zero energy wavefunctions for the Majorana fermions. We have delineated the region in parameter space where these solutions exist. In the uniform case, the two zero modes are peaked at the kink and anti-kink positions and are well separated if the kink and antikink are well separated. The analytic solutions also show how the zero mode wavefunctions can be engineered by tuning the couplings J_y and J_z in a site dependent way.

In conclusion our results show how zero energy Majorana modes can be created and manipulated in the tetrahedral spin chain if it is possible to tune the flux configurations and the local couplings. In this work, we have not addressed the interesting and important question as to how this is useful to braid unpaired Majorana modes. While this is of course not a meaningful operation in a chain, it may be possible to implement braiding in a network of coupled chains using the results obtained in this paper. We are pursuing this line of work and hope to report on it in future.

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